

Effect of nonlinearity on the dynamics of a particle in dc field-induced systems

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Abstract

Dynamics of a particle in a perfect chain with one nonlinear impurity and in a perfect nonlinear chain under the action of dc field is studied numerically. The nonlinearity appears due to the coupling of the electronic motion to optical oscillators which are treated in adiabatic approximation. We study for both the low and high values of field strength. Three different range of nonlinearity is obtained where the dynamics is different. In low and intermediate range of nonlinearity, it reduces the localization. In fact in the intermediate range subdiffusive behavior in the perfect nonlinear chain is obtained for a long time. In all the cases a critical value of nonlinear strength exists where self-trapping transition takes place. This critical value depends on the system and the field strength. Beyond the self-trapping transition nonlinearity enhances the localization.

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The application of dc field on a charge particle in a perfect periodic lattice would cause the oscillatory movement of the particle with frequency $\omega = eEa/\hbar$. Here e is the charge of the particle, a is the lattice spacing and E is the strength of the electric field. This oscillation is called Bloch oscillation [1]. The rapid oscillation of the charge particle may act as a fast emitter of electromagnetic radiation. However, the detection in bulk sample is almost impossible due to the fact that scattering time is much smaller than the period of Bloch oscillator. Esaki and Tsu [2] first studied the Bloch oscillation in superlattice structure (SL) which have long periods that makes the possible application for obtaining electromagnetic radiation in terahertz range. Recently these phenomena have been confirmed by various laboratory experiments [3]. A simple theoretical approach which captures the underlying physics is to use tight-binding models. Recently, the dynamical localization of a carrier has been studied in a one-dimensional perfect lattice with one linear impurity [4]. The resonance occurs for a particular value of the applied field and the strength of the impurity. This is observed only when the electric field is very high [5]. In this case the two on-site energies coincide which enhances the hopping of the carriers between the two degenerate sites. On the other hand, for weak field the degenerate sites are far apart from each other and as a result there is almost complete localization at the impurity site.

In this work we numerically study the dynamics of a charged particle in a linear chain with a single nonlinear impurity and in a perfect nonlinear chain under the action of dc electric field. The general equation of motion for the system is given as

$$i\hbar \frac{dc_m}{dt} = V(c_{m+1} + c_{m-1}) - (\epsilon_m + \chi_m |c_m|^2 + eamE)c_m. \quad (1)$$

Here $c_m(t)$ is the probability amplitude of the particle at site m at time t , V is the nearest-neighbor transfer matrix element, ϵ_m and χ_m are on-site energy and nonlinearity strength of the m -th site, respectively. Here, we assume $e = a = \hbar = V = 1$. The nonlinearity arises due to the coupling of quasiparticles with optical oscillators in adiabatic approximation [6]. When the electric field E is zero the equation is called one-dimensional discrete nonlinear Schrödinger equation (DNLS) [6–10]. The interesting property of DNLS equation is that

self-trapping transition occurs if the nonlinearity strength exceeds a critical value. The mean-square displacement (MSD) for perfect nonlinear systems [7] as well as random nonlinear systems [8,9] goes as $\sim t^2$. It has been found that the time-averaged site-probability is a good candidate to study the dynamics of the system [9,10]. So, we mainly study here the time-averaged probability of different sites of the systems discussed above for low as well as high electric field. The time-averaged probability at m -th site is defined as

$$\langle P_m \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |c_m(t)|^2 \quad (2)$$

with $|c_m(0)|^2 = \delta_{m,0}$. We solve the coupled nonlinear differential equations numerically using 4-th order Runge-Kutte method. To avoid the boundary effect we use self-expanding lattice [11]. For time-averaging we have taken $T = 2000$. The accuracy of numerical investigation is checked through the total probability. To examine the long time behavior of the system we also study the particle propagation and MSD. The MSD is defined as

$$\langle m^2 \rangle = \sum_{m=-\infty}^{\infty} m^2 |c_m(t)|^2 \quad (3)$$

with the same initial as above.

We first study the dynamical properties of a dc field-induced perfect chain containing only one nonlinear impurity at the zeroth site. The equation of motion is same as Eq. 1 with $\epsilon_m = 0$ for all m and $\chi_m = \chi \delta_{m,0}$. The nonlinearity alters the effective strength of the zeroth site dynamically as it depends on the occupation probability at that site. In a single linear impurity problem the degeneracy between the zeroth site and m th site occurs when $\epsilon_0 = mE$ (where ϵ_0 is the defect strength at zeroth site) [4,5]. But here, the degeneracy ($\chi |c_0(t)|^2 = mE$) may appear dynamically i.e. the strength of the zeroth site and any other site become equal at different instants of time. This is due to the oscillatory behavior of $|c_0(t)|^2$ with time t . For low field (e.g. $E = 0.5$) the time-averaged probability of a few sites as a function of nonlinearity strength χ is shown in Fig. 1. In this study we can define three regions of χ where the behavior changes significantly: (1) for small values of nonlinearity strength ($\chi < 3$) where we find smooth behavior of time-averaged probability

of the sites under study; (2) intermediate values of χ , ($3 < \chi < 4.8$) where we obtain small fluctuations and (3) high values of χ (> 4.8) where the particle is confined at the zeroth site with maximum probability. In region (1) for very small values of χ we do not find any significant change. However, if we increase the value of χ further particle gets confined towards the right side ($m > 0$) of zeroth site with maximum probability (see Fig. 2). Due to the presence of nonlinearity at zeroth site, it becomes dynamically degenerate with the sites right to the zeroth site. On the other hand, the energy difference between the zeroth site and its left neighbor ($m = -1$) is in general greater than the applied electric field. Consequently, the particle prefers to move towards $m > 0$. The MSD oscillates and its amplitude also changes with time. In region 2, the fluctuations occur due to the chaotic behavior of site-probabilities [10]. It should be noted that the values of $\langle P_m \rangle$ with $m \geq 0$ under study are almost equal. This implies particle localizes within a region uniformly. The region of localization depends on the dynamical degeneracy of the furthest site with the zeroth site (i.e. the site which is degenerate with zeroth site at time $t = 0$). This behavior is a sharp contrast to the linear impurity problem [4]. In linear impurity problem the particle gets localized at the defect site more and more with increasing the defect strength. In the fluctuation regime the value of MSD is even larger than that of perfect field-induced systems. Thus, the nonlinearity reduces field-induced localization. Beyond the fluctuations regime we find a self-trapping transition at $\chi_{cr} \sim 4.8$ where the maximum probability is gathered at the initial excitation site (i.e. zeroth site). Just below χ_{cr} , as χ increases the time spending by the particle at zeroth site with maximum probability also increases. This indicates the self-trapping transition at χ_{cr} . However, after χ_{cr} if we increase the value of χ the time-averaged probability of the zeroth site increases and of other sites it decreases. The value of MSD decreases even than that of field-induced perfect system. In the absence of electric field the self-trapping transition occurs at $\chi_{cr} \sim 3.2$ [9,10]. Thus, the value of χ_{cr} increases due to the presence of electric field. The particle has a tendency to move to the dynamical degenerate sites. Consequently, to get the self-trapping transition larger value of χ is required.

In Fig. 3 we have plotted the time-averaged probability of different sites as a function χ for high electric field (e.g. $E = 5$). Here, $\langle P_0 \rangle$ and $\langle P_1 \rangle$ initially decreases and increases respectively with increasing χ . Beyond $\chi \sim 7.7$ we find the fluctuations in the time-averaged probabilities. The self-trapping transition occurs at $\chi_{cr} \sim 12.1$. Without any nonlinearity the particle gets localized at the zeroth site with maximum probability. As we increase the value of nonlinearity the amplitude of the occupation probability of zeroth and its right neighbor site ($m = 1$) increases. Thus the time-averaged probability of these two sites decreases and increases respectively with increasing χ . In the fluctuation regime particle first gets localized within the sites $m = 0$ and 1 with maximum probability. Here, $|c_0(t)|^2 \leq 1$ and it has oscillatory behavior. So, to obtain the degeneracy ($\chi|c_0(t)|^2 = E$) between zeroth and its right neighbor site at many instants of time, the value of χ should be larger than E . This is exactly obtained. As we increase χ the site $m = 2$ also starts becoming degenerate with zeroth site at different instants of time. Thus $\langle P_2 \rangle$ gradually increases with increasing χ and at some values of χ we find $\langle P_0 \rangle$, $\langle P_1 \rangle$ and $\langle P_2 \rangle$ are almost equal. This means that the particle gets localized within the three sites $m = 0, 1$ and 2 . To find the long time behavior we also study the particle propagation. The behavior is consistent with that of time-averaged probability. It should be noted that in single linear impurity problem the resonance occurs between the two sites [4]. However, in the study of MSD we find the nonlinearity suppresses the field-induced localization as like low field case. Beyond χ_{cr} we find increasing of $\langle P_0 \rangle$ and decreasing of the time-averaged probability of all other sites with increasing χ . This means that the particle gets localized at the initial excitation site with maximum probability. The study of MSD shows the enhancement of the localization. It should be noted that the critical value of χ for self-trapping transition increases with increasing the strength of dc field. As we increase the field strength larger values of χ are required to get the degeneracy between the sites at many instants of time. The particle prefers to move to the degenerate sites. Consequently, larger χ values are required to get the self-trapping transition.

We now discuss the behavior of quasiparticles in field-induced perfect nonlinear chain. The equation of motion is same as Eq. 1 with $\chi_m = \chi$ and $\epsilon_m = 0$ for all m . The strength of

all the sites are altered dynamically depending on the probability of the corresponding sites. We first study for low field strength (e.g. $E = 0.5$). The time-averaged probability of a few sites as a function of χ is shown in Fig. 4. For small values of nonlinearity the time-averaged probability of the sites under study shows smooth behavior. We find that the dynamical localization gets destroyed even for small values of χ . However, particle gets localized within a few sites. For further increase of χ fluctuations, albeit small, in time-averaged probability of the sites under study occur. The fluctuation regime starts from $\chi \sim 2$. In this regime MSD shows subdiffusive behavior for a long time with many oscillations as shown in Fig. 5(a). The dynamic alteration of the site energies makes the localization weak. The oscillating behavior in MSD indicates the strong localization due to the applied electric field. Near the self-trapping transition we find particle initially gets localized at the initial excitation site for some time. Then it gets diffused to other sites. As we move towards the critical value of χ the particle gets trapped at the zeroth site for longer and longer time. This also reflects in the study of time-averaged probability. Two sharp falls in $\langle P_0 \rangle$ occur near χ_{cr} . Thus we get the self-trapping transition at $\chi_{cr} \sim 5.7$. It should be noted that the value of χ_{cr} of field-induced perfect nonlinear system is larger than that of single nonlinear problem (compare Fig. 1 and Fig. 4). In the former case the localization is weaker than the later one and consequently, to get the self-trapping transition more χ value is needed. However, above χ_{cr} nonlinearity enhances the field-induced localization.

In Fig. 6 we have plotted the time-averaged probability of a few sites of perfect nonlinear chain for high dc field (e.g. $E = 5$). For small values of χ they show smooth behavior. In this region the asymmetric particle propagation and oscillatory behavior in the amplitude of MSD is also obtained. For further increase of χ , the fluctuations in time-averaged probabilities occur. Due to the alteration of the site energies in this region ($6.9 < \chi < 12.68$) particle moves away from the site which is degenerate with the zeroth site at $t = 0$. Here also subdiffusive behavior in MSD is obtained for a long time as shown in Fig. 5(b). As the energy difference between the sites (due to the electric field) is large, the particle gets localized within a few sites with maximum probability. Thus the value of MSD is much

smaller than that of low field case. However, after self-trapping transition ($\chi_{cr} \sim 12.68$) we find the particle gets localized at the initial excitation site and consequently the value of MSD is smaller than that of perfect field-induced systems. Thus if χ exceeds the critical value where the self-trapping transition occurs nonlinearity makes the localization stronger.

In conclusion, our numerical study of the dynamics of the particle in a perfect chain with one nonlinear impurity and in a perfect nonlinear chain under the action of low as well as high electric field indicates the existence of three regions of χ where the behavior is different. The values of χ are different for different systems and field strengths. In all the cases we found a sharp self-trapping transition of $\langle P_0 \rangle$ at χ_{cr} . The critical value of χ depends on the system as well as field strength. When $\chi < \chi_{cr}$ the nonlinearity reduces the field-induced localization. Even we obtained subdiffusive behavior in field-induced perfect nonlinear systems. However, above the critical value of χ nonlinearity enhances the localization.

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FIGURES

FIG. 1. Plot of time-averaged probability $\langle P_m \rangle$ as a function of χ for different values of m in a perfect lattice containing a nonlinear impurity. The value of E is 0.5.

FIG. 2. Electronic probability propagation profile as a function of time (t) for $\chi = 2.5$ and $E = 0.5$ in the same system as in Fig. 1.

FIG. 3. Same as Fig. 1 but $E = 5$.

FIG. 4. Time-averaged probability $\langle P_m \rangle$ as a function χ for different values of m in a perfect nonlinear chain. Here $E = 0.5$.

FIG. 5. log-log plot of MSD as a function of time t of a perfect nonlinear system. (a) The solid curve corresponds to $E = 0.5$ and $\chi = 3.5$. (b) The dotted curve corresponds to $E = 5$ and $\chi = 11$.

FIG. 6. Same as Fig. 4 but $E = 5$.

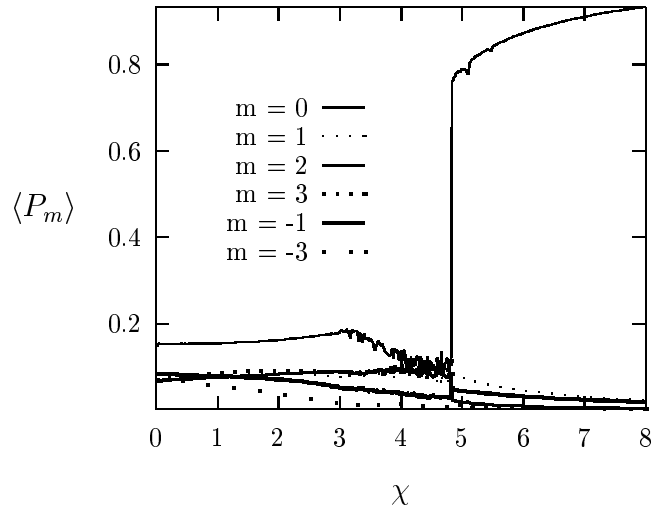
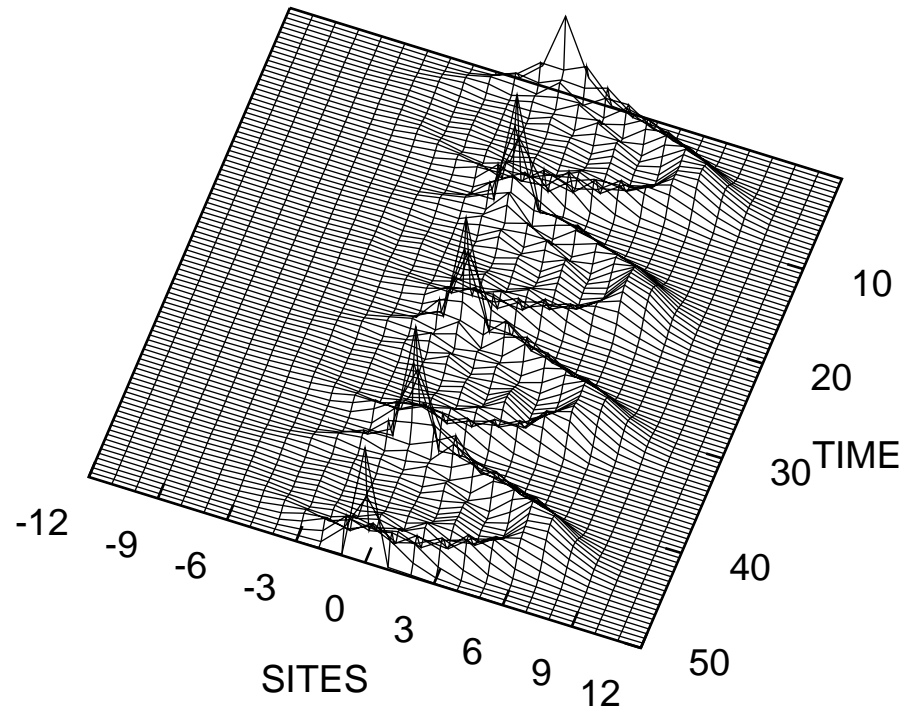


FIG. 1

FIG. 2



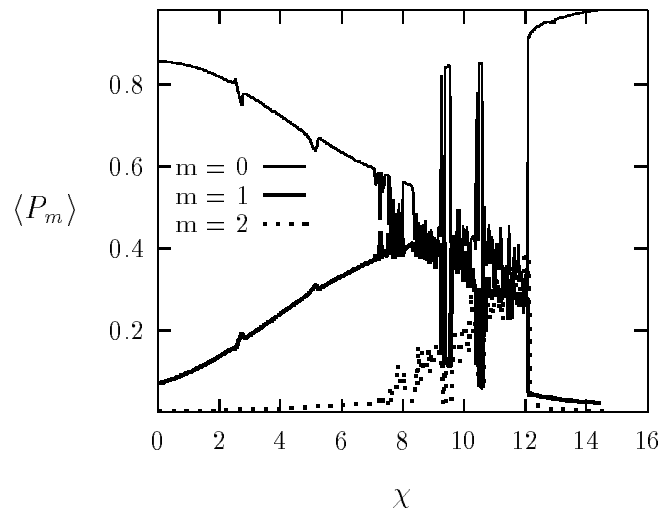


FIG. 3

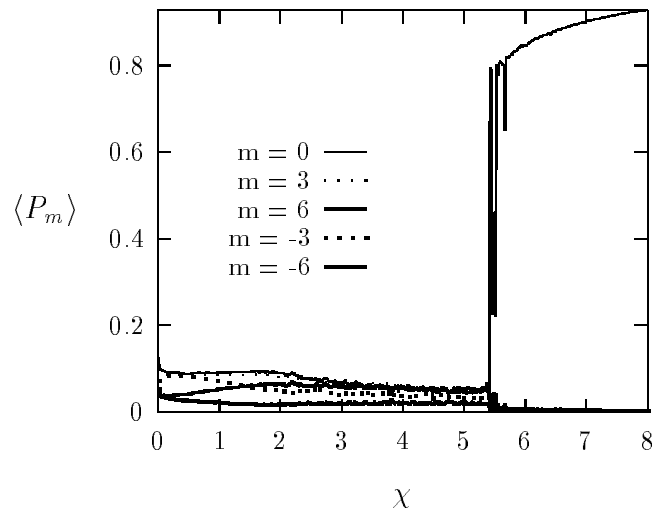


FIG. 4

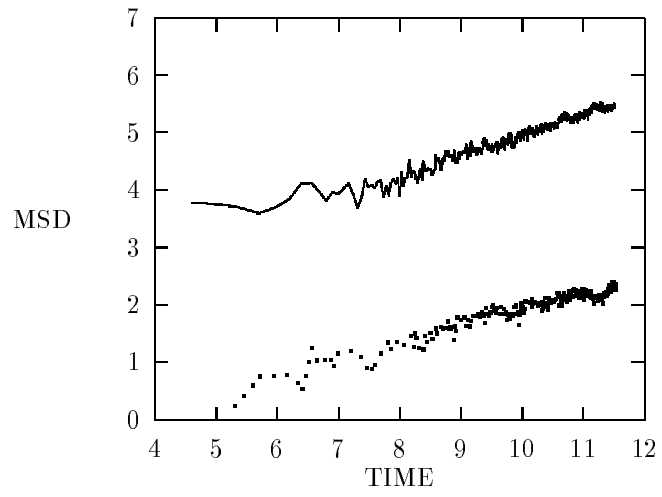


FIG. 5

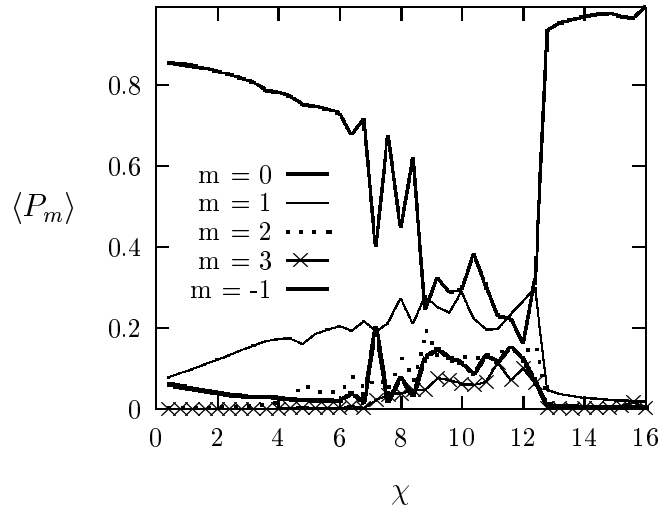


FIG. 6